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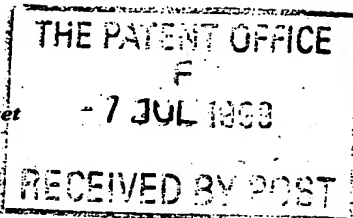
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2. Patent application number (The Patent Office will fill in this part)	07 JUL 1999		9915788.5
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Patents ADP number (if you know it)	2691002 ✓		
If the applicant is a corporate body, give the country/state of its incorporation	United Kingdom		
4. Title of the invention	Neural Network		
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**NEURAL NETWORK**

This invention relates to a neural network. Examples of the invention are described in the attached papers A,B  
5 and C.

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# A Novel Hybrid Neural Network for Identification of Trace Compounds

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## Abstract

Trace compound identification forms an important element of forensic science. Innovative instrumental designs based on Raman spectroscopy have made possible its *in-situ* use on fingerprint samples. Recently, the Pulse-Coupled Neural Network (PCNN), an oscillatory model neural network, has been used for invariant feature extraction for object recognition and classification. In this paper, we propose a novel hybrid neural network model for quick identification of trace materials from their Raman images. This network consists of a PCNN pre-processor. The features (icons) generated by the PCNN are then fed into a feedforward neural network for classification.

## 1. Introduction

Identification of prohibited trace compounds remains essentially the job of expert spectroscopists. Raman spectroscopy proves to be a versatile technique for analyzing and identifying such materials. It is fast, requiring little sample preparation time whilst being a non-destructive technique. Identification of trace compounds can be a cumbersome job since it implies cross-checking within a large database of Raman spectral bands and, more so, given the possibility that these may be present as mixtures.

Photons interact inelastically with atomic vibrations (phonons) to produce Raman scattered light. A given molecule will have a characteristic Raman spectrum - a unique fingerprint of a material. The whole Raman spectrum therefore contains information about the structure of the molecule and its environment. The amount of material required for Raman work can be as low as 1 picogram in mass. This has been recently demonstrated using the Renishaw Raman microscope [1], developed at Leeds. This innovative design has

enabled its *in-situ* use for imaging on fingerprint samples. The instrument has also been tested remotely using fibre optics with a view to develop portable Raman systems [2].

Neural networks are increasingly being used in several applications. There has been considerable interest in their use for pattern recognition. Recently, studies of the visual cortex of the cat highlight the role of temporal processing using synchronous oscillations for object identification [3]. This has led to a Pulsed-Coupled Neural Network (PCNN) wherein dendritic processing is incorporated through the use of multiplicative modulation along with a linking mechanism. This biologically inspired network is very well suited for image/signal pre-processing [4].

In this paper, a novel technique, involving a hybrid of a PCNN and a classical MLP feedforward network, is described for the purpose of quick identification of chemical compounds in trace amounts. Raman spectral images of these trace compounds are presented to the PCNN pre-processing unit to obtain outputs that are assembled into time signatures (or icons) of the specimen. The Multi Layer Perceptron (MLP) classifier is then trained by using a database of such icons. Preliminary results suggest this hybrid network has a great potential for the recognition of materials present in minute amounts.

## 2. The Hybrid Neural Network

An MLP classifier can be constructed directly from Raman spectra for the present objective. However, this will require a very large MLP with hundreds of input neurons. In our proposed method we use a hybrid neural network. This network consists of two sections:

- (a) a pre-processing PCNN that produces the Raman images' signatures, and
- (b) a post-processing neural network (a classical MLP) that will recognize the signature.

The PCNN, Figure 1, has received much attention from the image processing community. It comprises of a two-dimensional integrate and fire neurons with one neuron for each input pixel. The PCNN neuron consists of three parts:

- (1) The input unit (dendritic tree) includes the image pixel input (real value) as well as feedback (binary) inputs from surrounding neurons.
- (2) The linking and feeding branches merged together to compute the internal activation  $U$ . The integrated signals from the linking synapse plus an offset term of '1' are multiplied with the integrating signals from the feeding synapse to produce a membrane voltage  $U$ .
- (3) The pulse generator, compares the threshold value  $\Theta$  and  $U$ . If  $U > \Theta$ , then the PCNN output becomes equal to 1 and is reset to a maximum value  $V_\Theta$ , else the output is zero and  $\Theta$  is decreased exponentially by the time constant  $\alpha_\Theta$ .

The PCNN can be implemented by iterating the following equations:

$$F_{ij}[n] = \exp(-\alpha_F) F_{ij}[n-1] + S_{ij} + V_F \sum_M M_{ijM} Y_{ij}[n-1] \quad (1)$$

$$L_{ij}[n] = \exp(-\alpha_L) L_{ij}[n-1] + V_L \sum_M W_{ijM} Y_{ij}[n-1] \quad (2)$$

$$U_{ij}[n] = F_{ij}[n] (1 + \beta L_{ij}[n]) \quad (3)$$

$$Y_{ij}[n] = \begin{cases} 1 & \text{if } U_{ij}[n] > \Theta_{ij}[n-1] \\ 0 & \text{otherwise} \end{cases} \quad (4)$$

$$\Theta_{ij}[n] = \exp(-\alpha_\Theta) \Theta_{ij}[n-1] + V_\Theta Y_{ij}[n-1] \quad (5)$$

where  $S$  is the stimulus input (the pixel intensity),  $F$  and  $L$  are the feeding and linking inputs to the neuron and  $Y$  is the output. The other parameters include three potentials,  $V$ , and three decay constants  $\alpha$ , associated with  $F$ ,  $L$  and  $\Theta$ , respectively;  $\beta$  being the linking scaling constant. The interconnections in  $M$  and  $W$  are local Gaussians (dependent on the distance between the neurons).

If a digital image is applied as input to such a PCNN network, the network groups image pixels based on spatial proximity and brightness similarity, Kuntimad [5]. A two-dimensional input function can be mapped into a one-dimensional output function for e.g. time-series. Spatial averaging of neural responses gives a temporal output signal that is shown to be valid as a coding mechanism. The time signal  $G[n]$ , as computed by equation (6), is the number of "on pixels" in each iteration.

$$G[n] = \sum_{ij} Y_{ij}[n] \quad (6)$$

Since the PCNN provides a one-to-one correspondence between images and their time signatures (icons), it is opportune to exploit this property in this paper to create a database of another set of fingerprints from Raman spectra of trace compounds.

The PCNN unit described above is only a pre-processor and requires some task specific post-processing. In this work, the post-processing is carried out by a backpropagation neural network since the objective is to classify, and subsequently, to identify different trace compounds. A database of the icons of the trace compounds is used for the training/testing of the neural network classifier. The icons generated by using the PCNN from the Raman spectrum of any material in the database can then be matched by the MLP classifier with the corresponding signature within the large database for identification.

### 3. Results

The method described above is used for the identification of a few trace compounds: Pentaerythritol tetranitrate (PETN), dimethyl dinitrobutane (DMNB), 2,4,6-Trinitro toluene (TNT), 4-mononitrotoluene (4MNT), 3,4-dinitrotoluene (34DNT), heroin, and cocaine [6, 7]. Typical Raman spectra of these materials excited at ca. 244 nm and 633 nm with chemical structures also shown in the Figures 2 and 3 respectively.

A large number of iterations is required for each Raman image before a cyclic pattern becomes discernible in the time signature. Thus, a sampled time signature is employed to cover a representative portion of the cycle (100 iterations). Different time signatures were obtained for each Raman image for 16 different sets of PCNN parameters ( $\alpha$ 's,  $\beta$  and  $V$ 's).

For excitation at 244nm/633 nm, 80/55 signatures were used to train the feed forward neural network with the

following architecture: 3 input neurons, 10 hidden neurons and 3 output neurons. Each training data consists of gated PCNN time signature amplitudes and the output data (in the required output format corresponding to the compound). The remaining signatures (32/25) were used to test the MLP.

Our test results indicate a high success rate (>98.3%) for the identification.

#### 4. Conclusions

One-dimensional time signatures (icons) were obtained from Raman images (two-dimensional) of selected trace compounds by using a PCNN pre-processor. These icons are used as a fingerprint database for these materials to train a Multi Layer Perceptron classifier. The icon corresponding to the Raman image of a particular compound could then be identified (with high success rate).

Thus, the identification process using neural network avoids the consultation of huge listings of the Raman bands/Raman peak intensities altogether - saving time. It also saves the institution from an in-depth training on Raman spectroscopy of these materials. The identification can thus be performed by non-experts. Our preliminary results in this work demonstrate the effectiveness of the hybrid neural network, and hence, its potential for use in other similar areas.

Our investigations are being extended to include a larger number of chemicals, mixtures of chemicals, and to study the effect of noise and fluorescence or scattering background inherent in Raman images.

#### 5. Acknowledgements

We are grateful to Professor D. N. Batchelder for providing the Raman images and for fruitful discussions. We would like to acknowledge the University of Mauritius for providing the necessary facilities.

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## Spectral recognition using a modified Eckhorn neural network model

H.C.S. Rughooputh and S.D.D.V. Rughooputh

*Indexing terms: Image processing, neural networks, spectral recognition*

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Studies of the visual cortex of the cat highlight the role of temporal processing using synchronous oscillations for object identification. In this paper, the original neural network model of Eckhorn has been modified according to the proposal of Johnson and others and used for spectral recognition. The method developed turns out to be a much simpler, faster and elegant way of spectral recognition than reported elsewhere.

There has been considerable developments in the use Artificial Neural Networks to solve object recognition tasks. Based on the recent experimental findings of the visual cortex of the cat, there is evidence of synchronised neural activity in the brain and that temporal correlation of firing of neural assemblies could serve as a general coding mechanism for feature binding and pattern segmentation [1]. This has led to a computer-modelled cortex (pulsed coupled) neural network (PCNN) (Figure 1) [2] wherein dendritic processing is incorporated through the use of multiplicative modulation along with a linking mechanism. This biologically inspired network is very well suited for image/signal pre-processing.

Recently a one-dimensional PCNN has been used as a peak segmenter for spectral peak finding [3]. However, the method utilised is complicated (involving tens of thousands of iterations) and may not always yield satisfactory result. We develop here, using a similar neural network, a much simpler and elegant way of spectral recognition. The recognition involves first the conversion of spectral images into binary barcode-like images followed by an identification step. We present in this work a few examples where the recognition has been used for the identification of materials, for diagnostic purposes and for condition monitoring of electrical machines. We focus on identifying chemicals such as narcotics

and explosives from their Raman spectra, on diagnosis of heart condition from ECG signals and on condition monitoring of power transformers. We demonstrate that our approach is fast and robust and suits real-time tracking applications.

The PCNN offers tremendous advantages. It has the inherent ability to extract the fundamentals of the image and it simplifies the image to allow recognition engines to perform far easier task than is within their realm. If a digital image is applied as input to such a network, the network groups image pixels based on spatial proximity and brightness similarity, Kuntimad [4]. The network comprises of a two-dimensional array of integrate-and-fire neurons with one neuron for each input pixel. Each neuron receives input signals from a feeding synapse and a linking synapse. The former gets its inputs from other neurons whilst the linking synapse obtains its inputs from lateral and feedback connections, both synapses inducing decaying potentials. The integrated signals from the linking synapse plus an offset term of '1' are multiplied with the integrating signals from the feeding synapse to produce a membrane voltage that is compared to a local dynamic threshold. When this membrane potential exceeds the value of the dynamic threshold, the neuron fires to produce an output spike; consequently, the threshold is significantly increased. This value then decays until the neuron fires again.

The PCNN does not require any training or adjustment to extract the image fundamentals from the diverse set of imagery. Edges and segments are extracted at different iterations and segments can easily be seen over the course of a few iterations. Segment extraction occurs since groups of neurons in a similar state tend to pulse in unison. Edges are extracted as the autowave expands from these segments. In the original form, the PCNN neurons will lose the unison pulsing according to the texture of the input. So, in time, the segments will tend to separate according to the texture. Thus, the most important aspect of the PCNN performing these extractions is that it is an inherent quality of the PCNN

Furthermore, the PCNN provides a higher quality of performance and easy recognition (accomplished with the iterated 'binary' images). The full mathematical description of the PCNN can be obtained elsewhere [5].

We demonstrate our novel method on three different applications: (a) identification of trace compounds from their Raman spectra, (b) monitoring of cardiac cycle (ECG tracings), and (c) condition monitoring of power transformer from its transfer function spectra. Individual input spectra, in the form of gray level images are presented to the PCNN. As an example, we show in Figure 2, the Raman spectrum of an explosive (trace compound), dimethyl dinitrobutane (DMNB), the corresponding 8-bit gray level image and the binary images produced by the PCNN after iterations 1, 2, 7 and 8. Figure 3 shows the 8-bit gray level images and the binary images produced by the PCNN after iterations 1 and 7 for two trace compounds, ECG tracings and phase spectra of power transformers. There is a one-to-one correspondence between the barcode-like PCNN output and the corresponding input image. This feature is exploited in our spectral recognition technique. These barcodes can be used either singly (one iteration only) or in combination (more than one iteration) as explained below.

The first iteration PCNN output is converted into a binary codeword and stored in a look-up table (LUT). For the spectral recognition, the codeword is obtained from the corresponding spectrum and its Hamming's distances from all the codewords in the LUT are computed. The spectrum corresponding to the least Hamming distance gives the identity of the input. Ties in minimum Hamming distance are resolved by repeating the procedure using codewords generated from other PCNN iterations. In our present work, ties did not occur and the recognition rate success was 100%.

In summary, we have presented a very fast and robust method for spectral recognition. The PCNN provides a higher quality of performance with easier recognition using the iterated 'binary' images than other techniques. Our test results obtained using the neural network demonstrate that the approach is fast and robust making it suitable for real-time tracking applications in a wide variety of fields.

*Acknowledgements:* The authors would like to thank Professor J. M. Kinser for his help. It is a pleasure to thank the University of Mauritius for providing the necessary facilities.

25 June 1999

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*Electronic Letters***FIGURE CAPTIONS**

**Figure 1:** The PCNN pre-processor – a schematic representation

**Figure 2:** *Bottom:* Raman Spectrum of DMNB excited at 633 nm.  
*Top (from left to right):* Gray level image of DMNB and PCNN outputs (iterations 1, 2, 7 and 8).

**Figure 3:** *From top to bottom (see text):*  
Raman spectra of DMNB and Cocaine; ECG tracings of a normal heart and one with atrial fibrillation; Phase Spectra showing effect of short circuits : no shorted turns, 2 turns on high voltage winding shorted, and 2 turns on adjacent windings shorted.

# Biologically-inspired hybrid neural network for spectral identification, condition monitoring and diagnosis

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Recent experimental findings of the visual cortex<sup>1</sup> of the cat have shown evidence of synchronised neural activity in the brain, thus suggesting that temporal correlation of firing of neural assemblies could serve as a general coding mechanism for feature binding and pattern segmentation. This has led to a computer-modelled cortex (pulsed coupled) neural network<sup>2</sup> (PCNN) wherein dendritic processing is incorporated through the use of multiplicative modulation along with a linking mechanism. Since then, there has been considerable interest in the use of spike producing neurons to solve object recognition tasks in many fields<sup>3-5</sup>. This biologically inspired network is very well suited for image/signal pre-processing. In this paper, the original neural network model of Eckhorn<sup>1</sup> has been modified according to the proposal of Johnson<sup>2</sup> and used for spectral recognition of materials and objects, for condition monitoring of machines and for medical diagnosis. Applications thus range from chemistry, medical and forensic sciences, engineering to astrophysics. The method developed turns out to be much simpler, faster and more robust than methods reported in literature and it is also suitable for real-time applications in many fields.

Traditional image processing is generally based on a limited set of fundamental operations such as convolution of matrices. For most applications, only a few image features (e.g. textures, edges and segments) are important. The traditional method of recognising objects

within an image is through the use of a Fourier filter that works by matching the frequencies of the target with those of the input image. This Fourier filter system as well as others (e.g. neural networks, morphology, and statistical image processing) have been shown to have a number of serious drawbacks when it comes to real world applications.

The PCNN offers tremendous advantages: It has the inherent ability to extract the fundamentals of the image and it simplifies the image to allow recognition engines to perform far easier task than is within their realm. If a digital image is applied as input to such a network, the network groups image pixels based on spatial proximity and brightness similarity<sup>6</sup>. The network, shown in Figure 1, comprises of a two-dimensional array of integrate-and-fire neurons with one neuron for each input pixel. Each neuron receives input signals from a feeding synapse and a linking synapse. The former gets its inputs from other neurons whilst the linking synapse obtains its inputs from lateral and feedback connections, both synapses inducing decaying potentials. The integrated signals from the linking synapse plus an offset term of '1' are multiplied with the integrating signals from the feeding synapse to produce a membrane voltage that is compared to a local dynamic threshold. When this membrane potential exceeds the value of the dynamic threshold, the neuron fires to produce an output spike; consequently, the threshold is significantly increased. This value then decays until the neuron fires again. The full mathematical description of the PCNN can be obtained elsewhere<sup>5</sup>.

The PCNN does not require any training or adjustment to extract the image fundamentals from the diverse set of imagery. Edges and segments are extracted at different iterations and segments can easily be seen over the course of a few iterations. Segment extraction occurs since groups of neurons in a similar state tend to pulse in unison. Edges are extracted as the

autowave expands from these segments. In the original form the PCNN neurons will lose the unison pulsing according to the texture of the input. So, in time, the segments will tend to separate according to the texture. Besides, the PCNN provides a good performance and easy recognition (accomplished with the iterated 'binary' images rather than the original input)<sup>7</sup>.

Recently, a one-dimensional PCNN has been used as a peak-segmenter for spectral peak finding<sup>8</sup>. However, the method utilised is complicated (involving tens of thousands of iterations) and may not always yield satisfactory result. Of the various methods reported so far for the suggested applications, none give truly convincing results. We present here a much simpler and elegant way for conducting these tasks using a similar neural network preprocessor. The recognition involves the conversion of spectral images (in their grey level format) into binary barcode-like images by the PCNN preprocessor. This is followed by an identification step.

We demonstrate our novel technique on a few examples embracing different applications:

- (a) condition monitoring of power transformer from its transfer function spectra,
- (b) identification of chemical compounds from their infrared spectra,
- (c) identification of trace compounds (narcotics and explosives) from their Raman spectra,
- (d) monitoring of cardiac cycle, and
- (e) identification of pulsar profiles.

Individual input spectra in the form of 8-bit grey level images (Figure 2) are presented to the PCNN. In Figure 3, we show the corresponding binary images produced by the PCNN after iterations 1 and 7. There is a one-to-one correspondence between these barcode-like PCNN outputs and the corresponding input images. This feature is exploited for our



recognition/diagnosis/monitoring tasks. We note that these binary barcodes can be used either singly (one iteration only) or in combination (more than one iteration).

In a preliminary study<sup>9</sup>, we reported the use of a look-up table (LUT) for recognition. In the current study, we make use of a much faster technique for recognition using n-tuple (RAM) based neural network<sup>10</sup> instead of the LUT. The memory-based architecture of RAM-based neural networks provides many important features including one-shot learning and fast recall times. The architecture is basically a number of LUTs in parallel where each LUT is analogous to the weight matrix of a feedforward neural network. The speed and success rate for recognition are very encouraging.

Our technique involving the hybrid neural network (PCNN preprocessor and n-tuple RAM-based neural network) has successfully been used for the purpose of recognition, diagnosis and condition monitoring tasks. It provides a better performance with easier recognition than any other existing techniques. Our test results demonstrate that the approach is fast and robust making it suitable for real-time applications.

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*Nature***FIGURE CAPTIONS**

Figure 1: The PCNN pre-processor – a schematic representation

Figure 2: 8-bit grey level input images of (from left to right)

- (a) Transfer function spectra of power transformer showing effect of short circuits  
*no shorts; 2 turns on HV windings shorted; 2 turns on adjacent windings shorted*
- (b) Infrared spectra of chemical compounds  
*Cyclohexanone; Acetate fibre Avtex code 6941; Poly(isobutyl methacrylate)*
- (c) Raman spectra of trace compounds:  
*Heroin and Tri Nitro Toluene (TNT)*
- (d) ECG tracings of human heart  
*Heart with Atrial Fibrillation and Normal Heart*
- (e) Intergrated Pulsar profiles  
*1426-66 and 1133+16*

Figure 3: Corresponding Binary PCNN image pairs (iterations 1 and 7) of spectra from Figure 2 – from top to bottom.



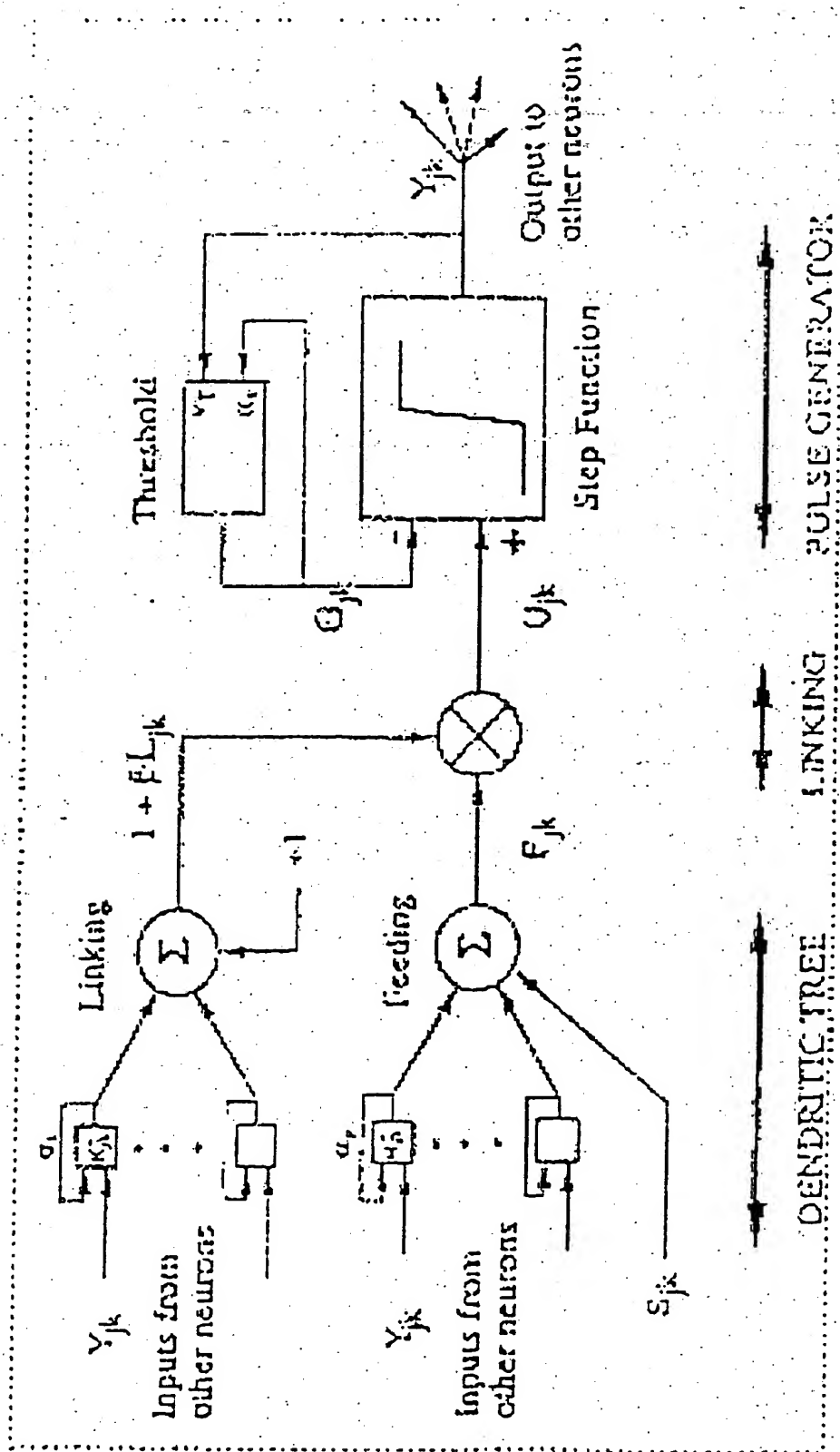


FIGURE 1: The PCNN pre-processor – a schematic representation



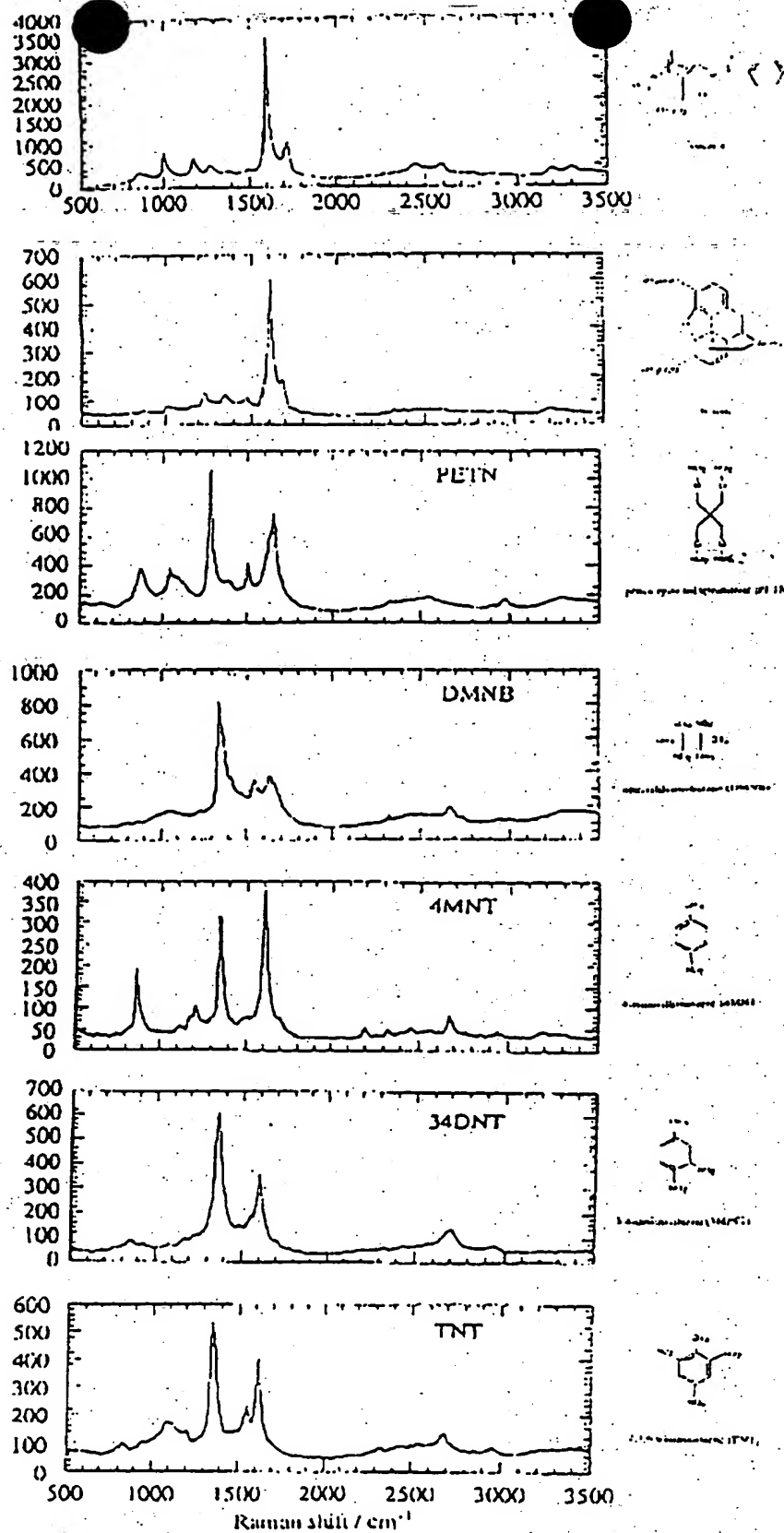


FIGURE 2: Raman Spectra of Narcotics & Explosives excited at 244 nm (with chemical structures)





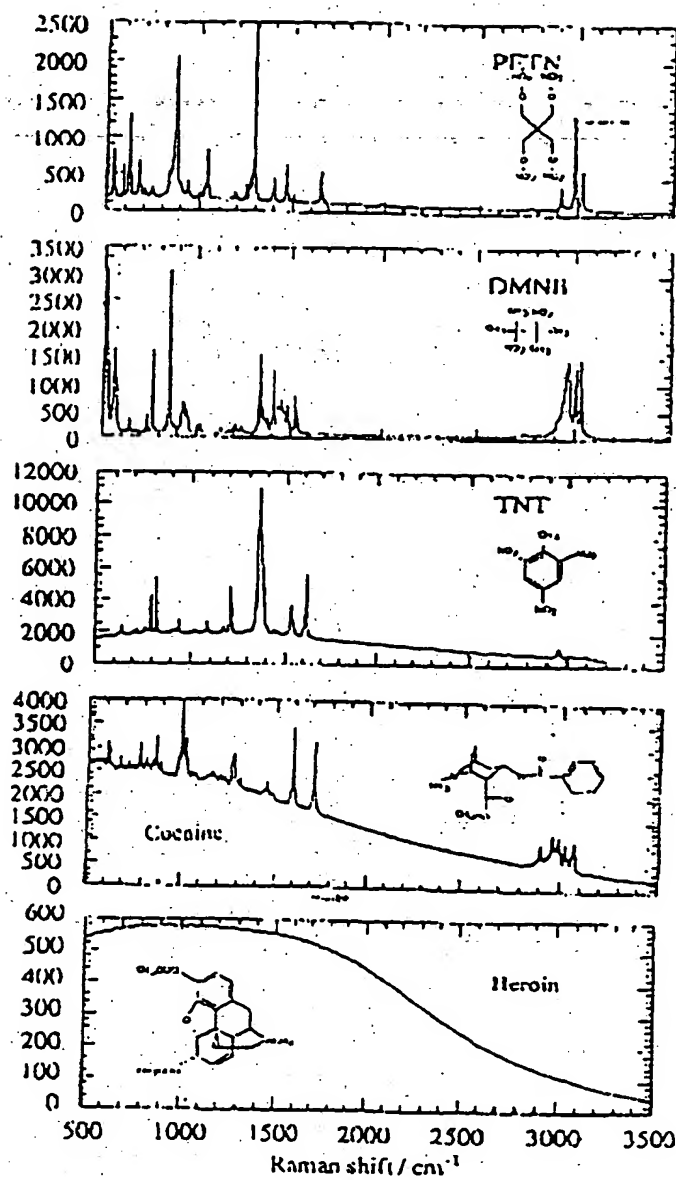


FIGURE 3: Raman Spectra of Narcotics & Explosives excited at 633 nm (with chemical structures)



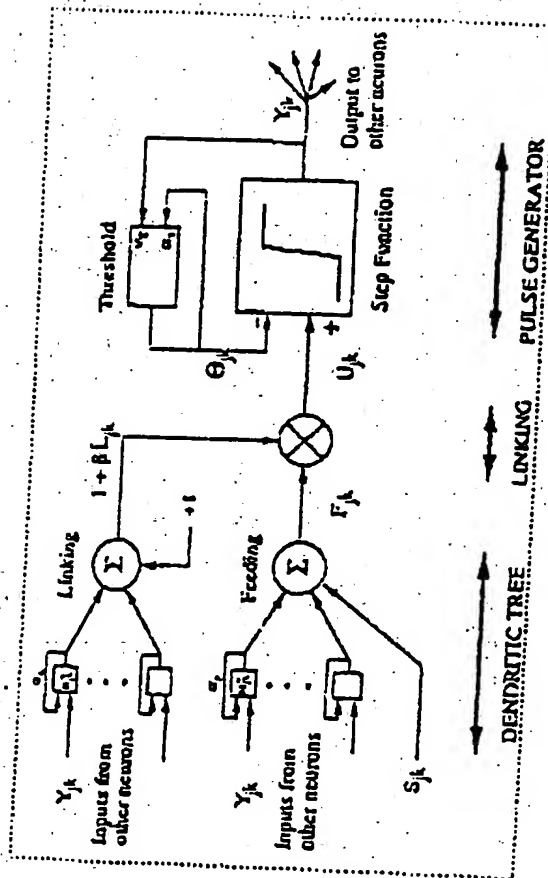


Figure 1: The PCNN pre-processor – a schematic representation



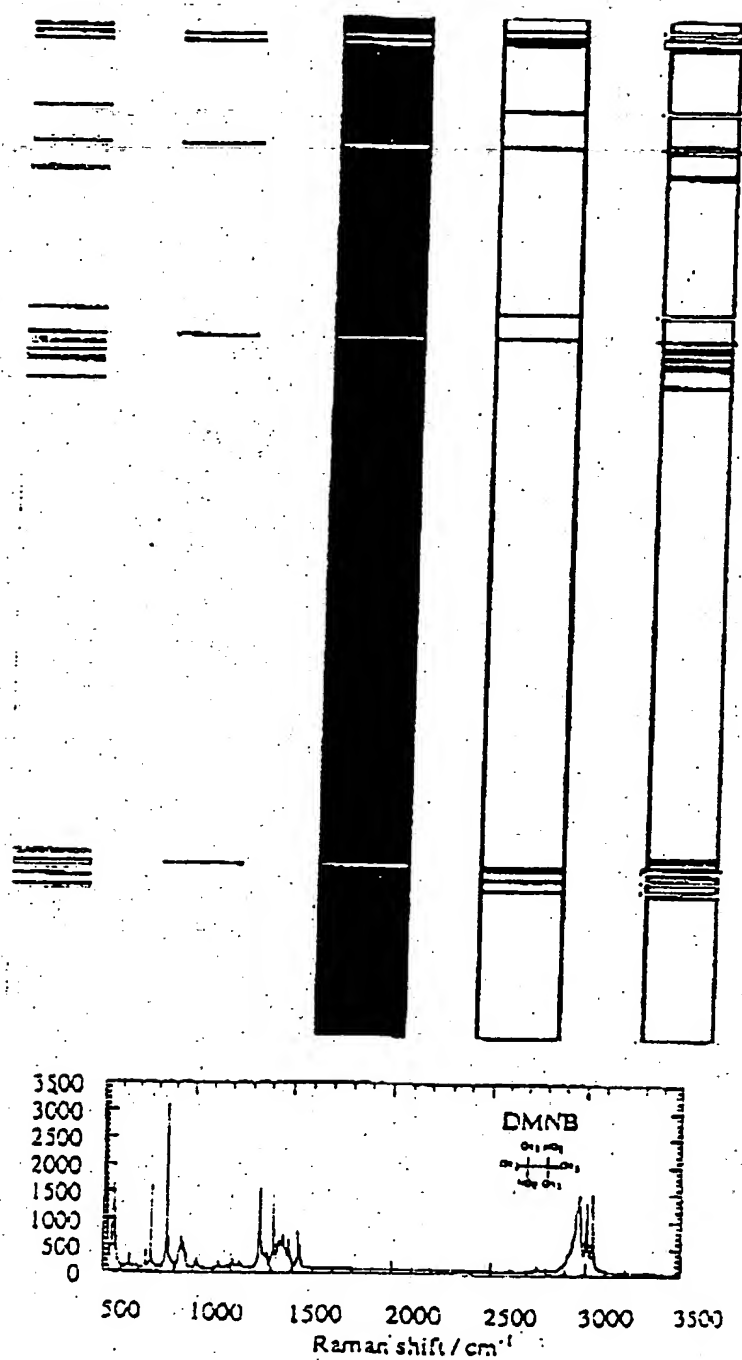


Figure 2: *Bottom:* Raman Spectrum of DMNB excited at 633 nm.  
*Top (from left to right):* Gray level image of DMNB and PCNN outputs (iterations 1, 2, 7 and 8).



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PAPER B

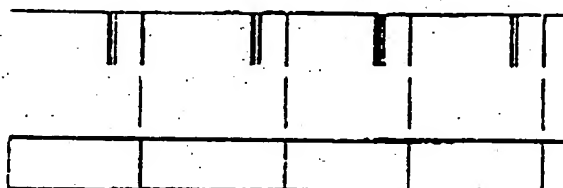
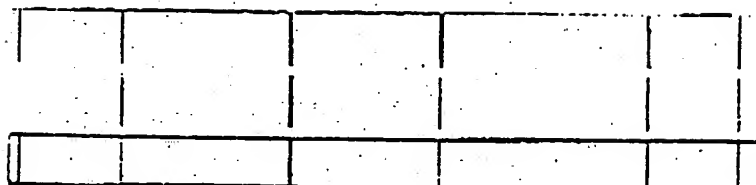
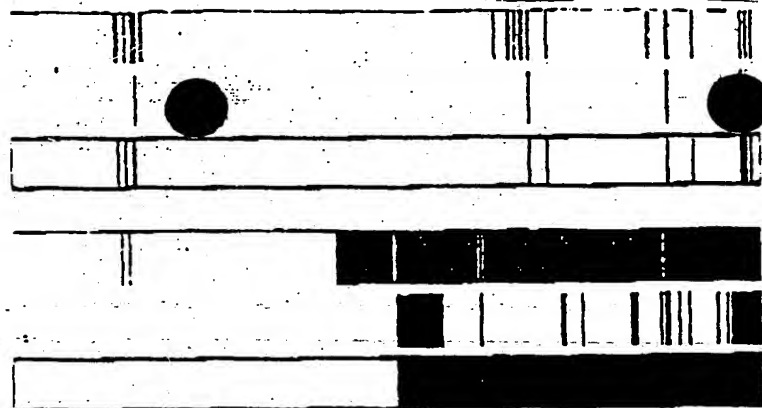


Figure 3: From top to bottom (see text):  
Raman spectra of DMNB and Cocaine; ECG tracings of a normal heart  
and one with atrial fibrillation; Phase Spectra showing effect of short  
circuits : no shorted turns, 2 turns on high voltage winding shorted, and 2  
turns on adjacent windings shorted.





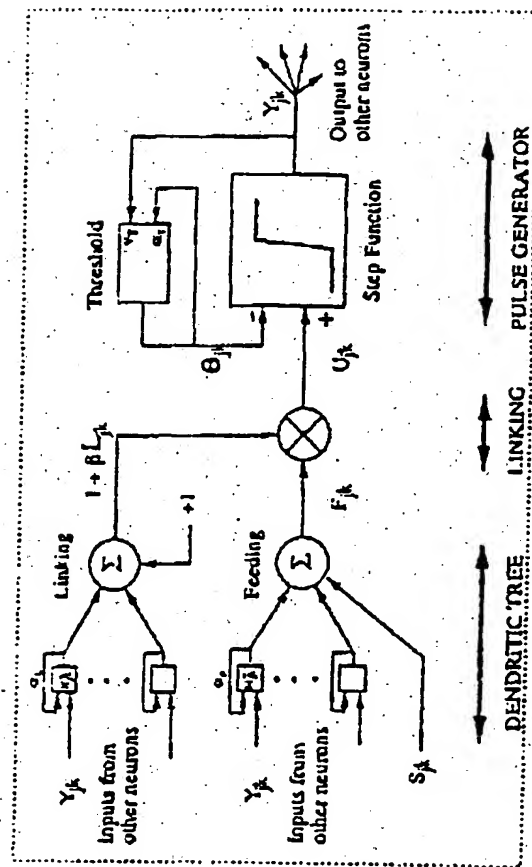


Figure 1: The PCNN pre-processor – a schematic representation



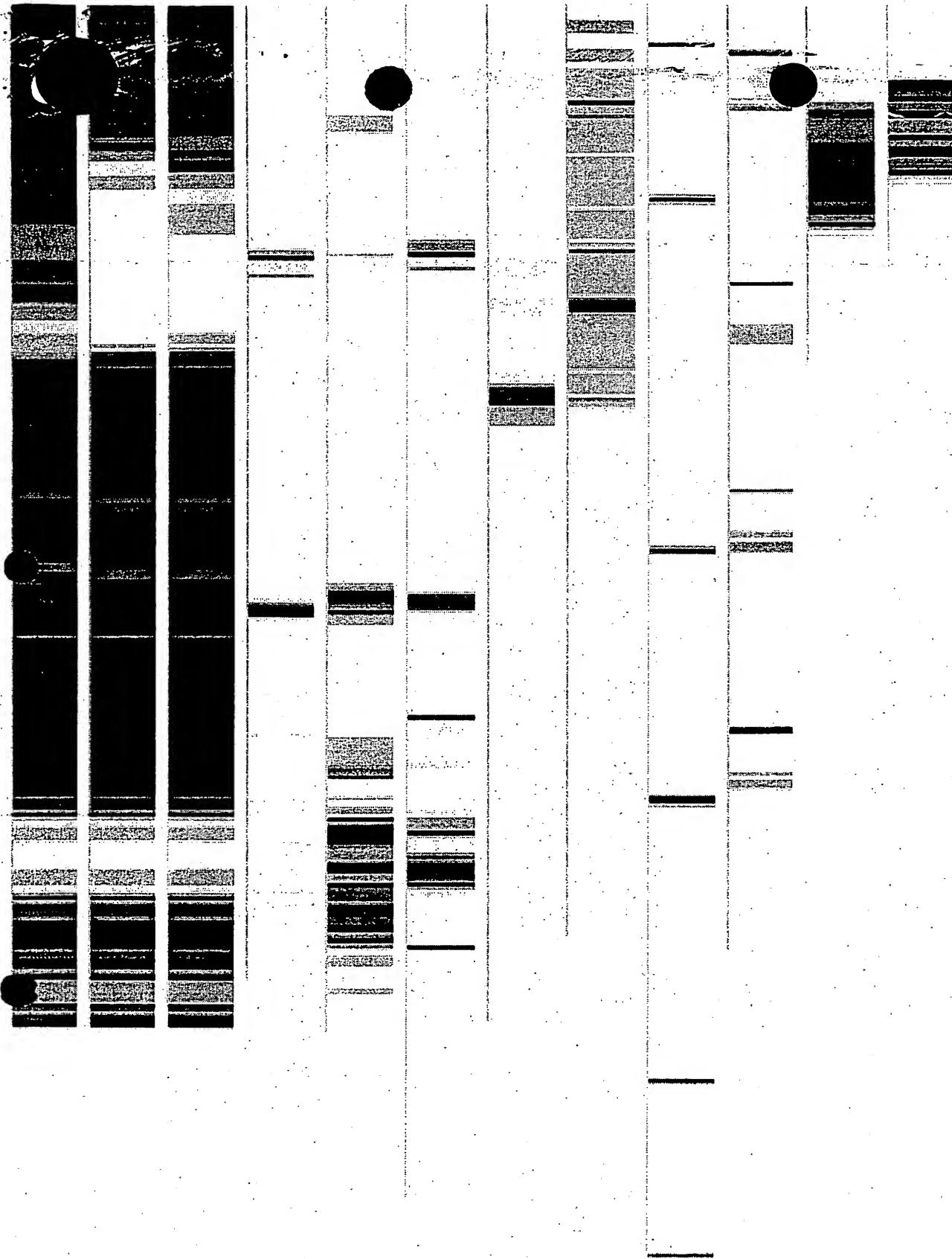


FIG 2



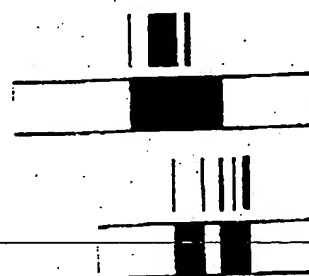
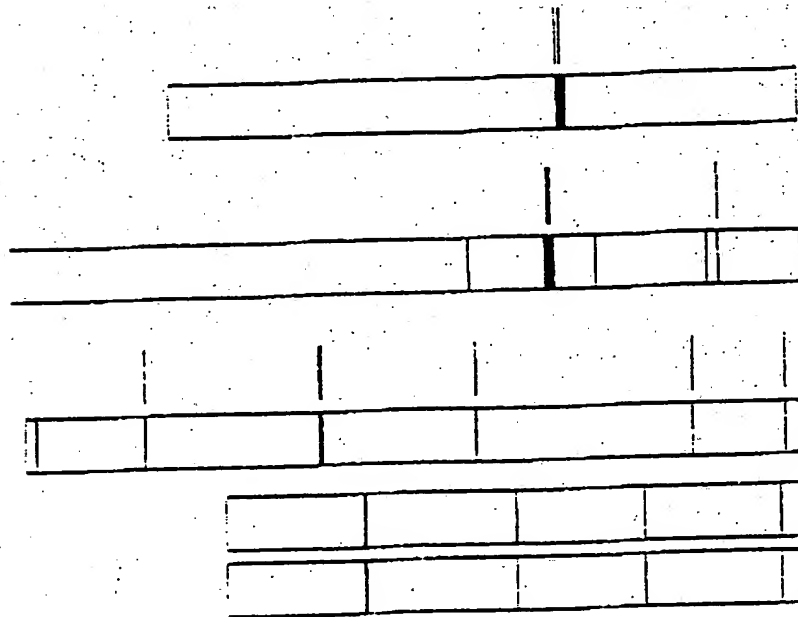
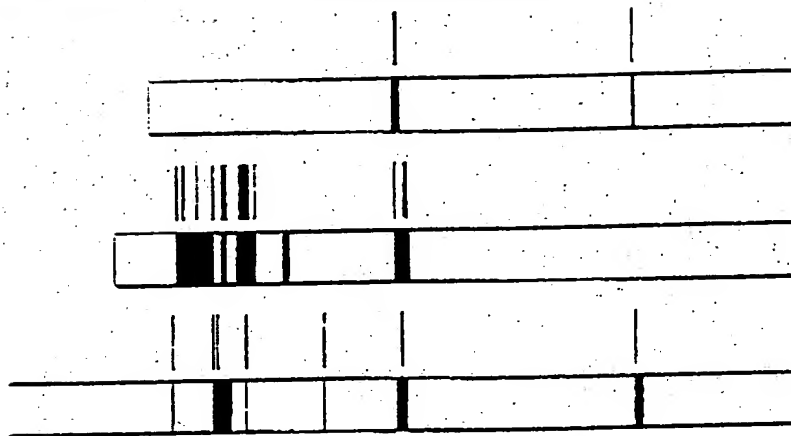


FIG 3

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